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Particles energy merging in 2D PIC codes

The effectiveness of Particle-In-Cell (PIC) codes in plasma dynamics simulation requires the ability to artificially change the number of particles during the calculation. The local number of particles per cell generally increases during the simulation and can be kept controlled in order to avoid exponentially increasing computation time ans to mantain a high enough local accuracy. The adopted technique is a spatial and energetic merging of the particles in the phase space based on conservation laws of total charge and energy and momentum of the two particles sets. In [1] a detailed description of the spatial merging was dealt with: particles inside the same cell can be merged together into two new particles positioned in order to conserve the charge fractions on the four cell nodes. Unfrtunately this is not enough: the new particles should conserve also the total energy and momentum of the starting ones and, in total, they should reproduce the same distribution function in the phase space. Few theoretical considerations will be given here about this topic.

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Abstract

The effectiveness of Particle-In-Cell (PIC) codes in plasma dynamics simulation requires the ability to artificially change the number of particles during the calculation. The local number of particles per cell generally increases during the simulation and can be kept controlled in order to avoid exponentially increasing computation time ans to mantain a high enough local accuracy. The adopted technique is a spatial and energetic merging of the particles in the phase space based on conservation laws of total charge and energy and momentum of the two particles sets. In [1] a detailed description of the spatial merging was dealt with: particles inside the same cell can be merged together into two new particles positioned in order to conserve the charge fractions on the four cell nodes. Unfrtunately this is not enough: the new particles should conserve also the total energy and momentum of the starting ones and, in total, they should reproduce the same distribution function in the phase space. Few theoretical considerations will be given here about this topic.

Contents

1 Introduction

In PIC simulations, merging techniques are required in order to reduce the particles number (and, consequently, the simulation time) where lower accuracy can be tolerated or when the number of particles per cell increases as a consequence of inonization events (only if a Monte-Carlo-Collisional (MCC) module is implemented). The reader is refered to [1, 2, 3, 4] if he's looking for more detailed information about the aims and advantages of particles merging technique in PIC codes.

The particles merging procedure consists in the replacement of a set of N particles of the same specieds with positions $\vec{x}_i$, velocities $\vec{v}_i$, charge q_i and mass m_i, with a different set

of $N' < N$ particles of the same type with positions $\vec{x}_{i'}$, velocities $\vec{v}_{i'}$, charge $q_{i'}$ and mass $m_{i'}$. The substitution must be based on the equivalence of the two ensembles, defined as the requirement that the two sets must represent the same physical system, with a different accuracy.

In kinetic PIC codes, two sets of particles can be considered equivalent if the following two conditions are satisfied:

- the two ensembles equally contributes to the grid moments appearing indistinguishable;

- the two sets sample the same velocity distribution function.

The first condition was already examined in [1] and two algorithms were proposed in [5]: for an electrostatic PIC code, the conservation of the charge fractions (zero-order moments in $\vec{v}$) on the grid nodes makes the two sets of particles appear indistinguishable from the poin of view of the electric field solver.

The second condition inevitably increases the variance of the statistical description of the distribution function. Therefore, the procedure has to be applied with care by merging particles near in velocity components and energy.

2 Momentum and energy conservation

Two-dimensional PIC codes follows particles with two position coordinates and three components of velocities (or two components plus total energy). When merging N particles, the momentum must be conserved in all its components and total energy as a scalar. Labelling the new N' particles with the prime, the conservation laws can be written as

$$\sum_{i=1}^{N} m_i v_{j,i} = \sum_{i'=1}^{N'} m_{i'} v_{j,i'} = M_j \qquad \text{with } j = 1,2,3$$
$$\sum_{i=1}^{N} \frac{1}{2} m_i \sum_{j=1}^{3} v_{j,i}^2 = \sum_{i'=1}^{N'} \frac{1}{2} m_{i'} \sum_{j=1}^{3} v_{j,i'}^2 = E\,,$$

where v_j with $j = 1,2,3$ are the three components of velocity, M_j the total momentum in the j-th direction and E the total energy of the set. Even if the conservation of the third component of momentum is neglected and the third velocity component is randomly extracted in order to allow energy conservation, 3 equations are obtained.

It was showed in [1] that $N' = 2$ particles are enough to replace a generic set of N particles pertaining to the same cell, preserving charge fractions on the nodes. Therefore, it's wise to assume $N' = 2$ even in this case, with a consequent degree of freedom for one of the 4 unknowns, i.e. the velocity components. To avoid this arbitrariness, the system can be closed considering conservation of each momentum component and of energy in each

direction, even if not strictly necessary. The resultant system is then rewritable as

$$m_{1'}v_{j,1'} + m_{2'}v_{j,2'} = \sum_{i=1}^{N} m_i v_{j,i} = M_j \qquad \text{with } j = 1,2,3 \tag{1a}$$

$$m_{1'}v_{j,1'}^2 + m_{2'}v_{j,2'}^2 = \sum_{i=1}^{N} m_i v_{j,i}^2 = 2E_j \qquad \text{with } j = 1,2,3\,. \tag{1b}$$

Moreover, the spatial merging already conserves the total mass of the system, since the ratio q/m must be preserved for each species apart of the particle weight. The mass m_i of the i-th generic particle is given by $m_i = w_i m$, where m is the mass of the particle species; then, the mass conservation can be simply written in terms of particles weights as

$$\sum_{i=1}^{N} m_i = m \sum_{i=1}^{N} w_i = mw\,,$$

where w is the total weight of the considered set of particles, and mw their total mass. To make the (1) dimensionless, each mass m_i can be divided by the total mass mw and each velocity component $v_{j,i}$ by the ratio of the total momentum and total mass $M_j/(mw)$, obtaining

$$\omega_{1'}\nu_{j,1'} + \omega_{2'}\nu_{j,2'} = 1 \qquad \text{with } j = 1,2,3 \tag{2a}$$

$$\omega_{1'}\nu_{j,1'}^2 + \omega_{2'}\nu_{j,2'}^2 = \varepsilon_j \qquad \text{with } j = 1,2,3\,, \tag{2b}$$

where

$$\omega_i = \frac{m_i}{mw} = \frac{w_i}{w} \qquad \nu_{j,i} = mw\frac{v_{j,i}}{M_j} \qquad \varepsilon_j = 2mw\frac{E_j}{M_j^2}\,.$$

Extracting $\nu_{j,2'}$ from (2a) and substituting it into (2b), a quadratic equation in $\nu_{j,1'}$ is obtained, having

$$\nu_{j,1'} = 1 \pm \sqrt{\frac{\omega_{2'}}{\omega_{1'}}(\varepsilon_j - 1)}\,, \tag{3}$$

as possible solutions (note that the relation $\omega_{1'} + \omega_{2'} = 1$ have been extensively used). The velocity components of the particle $2'$ are derived by (2a):

$$\nu_{j,2'} = \frac{1}{\omega_{2'}}(1 - \omega_{1'}\nu_{j,1'}) = 1 \mp \sqrt{\frac{\omega_{1'}}{\omega_{2'}}(\varepsilon_j - 1)}\,. \tag{4}$$

Note that the weight fractions $\omega_{1'}$ are defined by the spatial merging procedure [1]; in particular, for equally weighted merging particles (the reader is referred to the first method presented in [1]), the ratio $\omega_{1'}/\omega_{2'}$ is equal to 1, leading to simplified expressions.

Looking at (3) and (4) it arises necessary to show that $\varepsilon_j - 1 \geq 0$ in order to obtain real valued $\nu_{j,1'}$ and $\nu_{j,2'}$. The mentioned condition is equivalent to

$$2mw\frac{E_j}{M_j^2} \geq 1\,;$$

multiplying both hands by $M_j^2 \geq 0$ and applying the definition of E_j and M_j for the initial set of N particles, the relation becmoes

$$\sum_{k=1}^{N} w_k \sum_{i=1}^{N} w_i v_{j,i}^2 \geq \left(\sum_{i=1}^{N} w_i v_{j,i} \right)^2 .$$

The square terms of the rhs equal the terms of the lhs for $k = i$, then teh two summations can be simplified in

$$\sum_{k=1}^{N} \sum_{i=1, i\neq k}^{N} w_k w_i v_{j,i}^2 \geq 2 \sum_{k=1}^{N} \sum_{i=k}^{N} w_k w_i v_{j,k} v_{j,i} = \sum_{k=1}^{N} \sum_{i=1, i\neq k}^{N} w_k w_i v_{j,k} v_{j,i} \,;$$

moving all the terms to the lhs, the relation can be simply written as

$$\sum_{k=1}^{N} \sum_{i=1, i\neq k}^{N} w_k w_i v_{j,i} (v_{j,i} - v_{j,k}) \geq 0 \,.$$

Adding the generic terms given by the couple of indexes $k = l$, $i = n \neq l$ and $k = n$, $i = l \neq n$, the generic addendum $w_l w_m (v_{j,l} - v_{j,m})^2$ is obtained. Therefore, the disequation containing the double summation assumes the form

$$\sum_{k=1}^{N} \sum_{i=k}^{N} w_k w_i (v_{j,k} - v_{j,i})^2 \geq 0 \,,$$

which is evidentely verified being the summation of positive terms.

It's, finally, trivial to go back from (3-4) to the real velocity components:

$$v_{j,1'} = \frac{M_j \pm \sqrt{\dfrac{m_{2'}}{m_{1'}} \left(2(m_{1'} + m_{2'}) E_j - M_j^2 \right)}}{m_{1'} + m_{2'}}$$

$$v_{j,2'} = \frac{M_j \mp \sqrt{\dfrac{m_{1'}}{m_{2'}} \left(2(m_{1'} + m_{2'}) E_j - M_j^2 \right)}}{m_{1'} + m_{2'}} \,.$$

Three random numbers can be extracted to fix the plus or minus sign of the three square roots in $v_{j,1'}$ for $j = 1, 2, 3$, those of $v_{j,2'}$ being the opposite. For example, the second term could be multiplied by $(-1)^{\mathrm{nint}(R)}$, with $\mathrm{nint}(R)$ the nearest integer of the random number R chosen in $[0, 1]$ with a uniform distribution.

3 Particles choice and energy binning

As already stated, the N particles chosen to undergo a merging procedure must be of the same species; moreover, to the induced error is reduced by selecting near particles in the

phase space. From the spatial point of view, the phase space can be considered already meshed by the grid of the PIC method: only particles pertaining to the same cell are chosen to conserve charges on the nodes as forseen by the spatial merging procedure. On the other hand, velocity components are treated continuously by the PIC codes; an additional method to select near particles in the 3D velocity domain has, then, to be formulated.

In a two-dimensional code, only two components of momentum plus the total energy are strictly essential. This means that the third component of velocity can be replaced by the total energy of the particle. The first two components of velocity, divided by the velocity magnitude in the (v_1, v_2) plane, give a planar direction of motion. The total energy, instead, gives information about the third velocity component.

The direction of flight ϑ_i of the i-th particle in the 2D domain is given by

$$\frac{v_{1,i}}{v_{1,i}^2 + v_{2,i}^2} = \cos\vartheta_i$$
$$\frac{v_{2,i}}{v_{1,i}^2 + v_{2,i}^2} = \sin\vartheta_i \,,$$

while its energy can be used to define a sort of distance from the origin of the polar system. When a MCC module is coupled to the PIC code to tochastically simulate collisions between charged species and a neutral background gas, the simulation weighted particles are treated as real particles when the collisions are modelled by sampling energy dependent cross sections. To avoid a biased solution, it's important to avoid weighting the energies through the particles mass until the new velocities have to be calculated from (1): a merging technique based on the energy of the weighted simulation particle would induce to select particles of apparently similar energies, which in the MCC module would become completely different loosing representativeness of the sample in the sthocastic modelling of threshold collisions (refer to [**?**] for similar considerations related to splitting techniques). Therefore, the quantity

$$\frac{2E_i}{m_i} = \left(v_{1,i}^2 + v_{2,i}^2 + v_{3,i}^2\right) = \varrho_i$$

is defined to discriminate particles for their energy and 3$^{\text{rd}}$ velocity component.

Each particle can then be placed in the plane on the basis of its angle ϑ and of the radius E_i of its corresponding trigonometric circle. A proper angular discretization allows to find particles with similar direction of flight, while an energetic binning groups particles with similar energies as if they were real particles (as from the point of view of the MCC module). A graphical representation can be of help: in figure 1), the plane (v_1, v_2) (here equivalent also to (x_1, x_2)) is represented; note that the isolines at different radiuses are not defined simply by $\sqrt{v_{1,i}^2 + v_{2,i}^2}$, but through $\varrho_i = \left(v_{1,i}^2 + v_{2,i}^2 + v_{3,i}^2\right)$ in a not totally consistent way. Merging particles pertaining to the same cell of the meshed polar space, the two-dimensional direction of flight and the total energy are roughly preserved. Increasing the number of cell towards a more refined mesh leads to a lower induced error, but, on the other hand, makes more difficult to find similar particles to be grouped toghether. A compromise must be found between a sufficiently low error and an advantageous effectiveness of the procedure.

Once merged, the new particles will lie in the same cell of the starting particles.

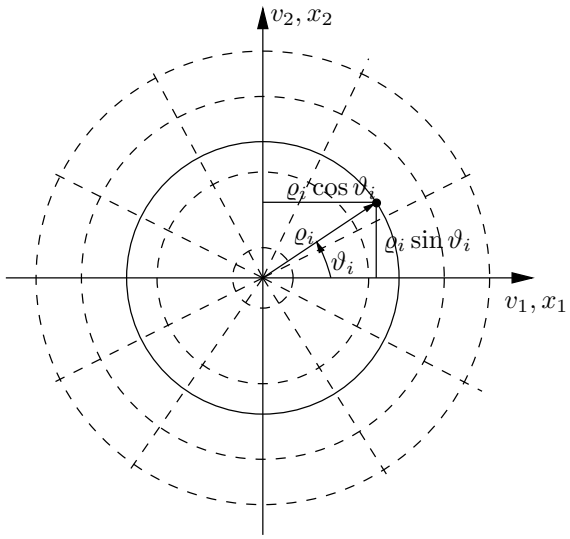

Figure 1: Bidimensional representation of particles distribution in 3D velocity space through their direction of flight and total unweighted energy. The dashed lines defines a polar mesh for the particles grouping.

4 Concluding remarks

In this brief report, the energetic merging in PIC codes is discussed. Combining it with the spatial merging already discussed in [1] a complete procedure is obtained for the whole phase space: once found a set of $N > 2$ particles near in space (inside the same cell) and with similar two-dimensional momentum components plus scalar energy, they can be merged toghether in $N' = 2$ particles exactly preserving charges on the cell nodes, conserving the total momentum and roughly reproducing the initial energy distribution function. Reducing the number of particles increases the variance on their distribution in the phase space and introduces errors related to momentum and energy discretization, but allow to reduce the overall computation time.

The criterion for the application of the merging technique will be subject of future works; moreover, the coupling of the merging procedure with a splitting one is of great importance to mantain a roughly constant number of particle per cell and a constant energetic density of the particles to have a good sampling of the distribution function.

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